AMENDMENTS TO THE CLAIMS

This listing of claims will replace all prior versions and listings in this application.

Listing of Claims:

1-22. (canceled)

23. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein the structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

24-26. (canceled)

27. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

28. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

29. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein the structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

30. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

31. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 characterize the binding pocket, and wherein the

homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

32. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein the structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) determining structure coordinates of inosine monophosphate dehydrogenase ("IMPDH") amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414,

415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

33. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

34. (previously presented) A method for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex, or a homologue of said binding pocket, with a deformation energy not greater than about 10 kcal/mole, wherein structure coordinates of IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 characterize the binding pocket, and wherein the homologue of said binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å comprising the steps of:

a) determining structure coordinates of IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1 to characterize the binding pocket;

b) employing computational means which utilize all or part of said structure coordinates and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

c) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

d) outputting said quantified deformation energy to a suitable output hardware; and

e) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

35 and 36. (canceled)

37. (previously presented) The method of claim 32, wherein the docking of the chemical entity with all or part of the binding pocket utilizes shape complementarity or is followed by molecular dynamics or energy minimization.

38. (currently amended) The method according to any one of claims 23, 29 or 32, further comprising the steps of:

[[e]]f) contacting the selected chemical entity with the molecule or molecular complex; and

[[f]]g) selecting the chemical entity that inhibits the catalytic activity of the molecule or molecular complex.

39. (canceled)

40. (previously presented) The method of claim 32, wherein the docking of the chemical entity with all or part of the binding pocket includes visual inspection on a computer screen using a computer program capable of generating a three-dimensional graphical representation of said structure coordinates and structure coordinates of said chemical entity.

41. (withdrawn) The method according to claim 23, 27 or 28, further comprising the steps of:

[[e]]f) repeating steps a) to [[d]]e) with a second chemical entity that associates with all or another part of said binding pocket, or homologue thereof;

[[f]]g) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

[[g]]h) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

42 and 43. (canceled)

44. (withdrawn) The method according to claim 29, 30 or 31, further comprising the steps of:

[[e]]f) repeating steps a) to [[d]]e) with a second chemical entity that associates with all or another part of said binding pocket, or homologue thereof;

[[f]]g) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

[[g]]h) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

45 and 46. (canceled)

47. (withdrawn) The method according to claim 32, 33 or 34, further comprising the steps of:

[[e]]f) repeating steps a) to [[d]]e) with a second chemical entity that associates with all or another part of said binding pocket, or homologue thereof;

[[f]]g) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

[[g]]h) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

48-62. (canceled)

63. (currently amended) The method of any one of claims 23, 29[[,]] and 32 ~~and 35~~ wherein the method is for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex with a deformation energy not greater than about 7 kcal/mole and step d) comprises selecting the chemical entity if said deformation energy is not greater than 7 kcal/mole.

64-71. (canceled)

72. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

73. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

74. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of said binding pocket structure coordinates defined by IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

75. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

76. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

77. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385,

386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

78. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

79. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a

deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

80. (new) A method for selecting a chemical entity that associates with all or part a binding pocket of a molecule or molecular complex of inosine monophosphate dehydrogenase ("IMPDH"), or a homologue thereof, with a deformation energy not greater than about 10 kcal/mole, wherein said homologue of said IMPDH binding pocket has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

a) employing computational means which utilize all or part of structure coordinates of said binding pocket defined by IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, and structure coordinates of the chemical entity, to dock the chemical entity with all or part of said binding pocket or homologue thereof;

b) quantifying the deformation energy between the chemical entity and all or part of the binding pocket or homologue thereof;

c) outputting said quantified deformation energy to a suitable output hardware; and

d) selecting the chemical entity if said deformation energy is not greater than about 10 kcal/mole.

81. (new) The method of any one of claims 72, 75 and 78, wherein the method is for selecting a chemical entity that associates with all or part of a binding pocket of a molecule or molecular complex of IMPDH, or homologue thereof, with a deformation energy not greater than about 7 kcal/mole and step d) comprises selecting the chemical entity if said deformation energy is not greater than 7 kcal/mole.

82. (new) The method of claim 78, wherein the docking of the chemical entity with all or part of the binding pocket utilizes shape complementarity or is followed by molecular dynamics or energy minimization.

83. (new) The method according to any one of claims 72, 75 or 78, further comprising the steps of:

e) contacting the selected chemical entity with the molecule or molecular complex; and

f) selecting the chemical entity that inhibits the catalytic activity of the molecule or molecular complex.

84. (new) The method of claim 78, wherein the docking of the chemical entity with all or part of the binding pocket includes visual inspection on a computer screen using a computer program capable of generating a three-dimensional graphical representation of said structure coordinates and structure coordinates of said chemical entity.

85. (new) A method for designing an IMPDH inhibitor, comprising docking a chemical entity with all or part of a binding pocket defined by IMPDH amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, wherein the docking of the chemical entity with all or part of the binding pocket utilizes shape complementarity or is followed by molecular dynamics or energy minimization.